Calibration of Oil Reservoir Simulation Codes

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What is the meaning of calibration?

Given a model of a physical system, calibration means:

- frequentist: estimation of model parameters
- Bayesian: inference of model parameters
Motivating application

What is the problem?
• maximizing economic recovery of hydrocarbons from subsurface reservoirs

What’s available?
• models of the reservoirs
• geophysical data gathered on site
Example - Umiat oil field
Oil reservoir simulator

Eclipse oil reservoir simulation software by Schlumberger
Oil reservoir simulator

Reservoir simulator principles:

- conservation of energy and mass
- isothermal fluid phase behavior
- Darcy approximation (fluid flow through porous media):

\[ Q = -\frac{kA}{\mu} \left( \frac{P_2 - P_1}{L} \right) \]

- \( k \) permeability, \( \mu \) viscosity
- \( Q \) discharge rate (\( m^3/s \))
The problem - Oil reservoir model

- 2D $100 \times 12$ grid blocks (Tavassoli et al. 2004)
- Three parameters:
  - poor quality sand permeability ($k_{low}$)
  - good quality sand permeability ($k_{high}$)
  - discontinuity (throw)
The problem - Oil reservoir model

- running time of the 2D oil reservoir model in Tavassoli et al. (2004): couple of seconds
- more complex and realistic 3D models - hours/days to run
Calibration of simulators

- We aim at inferring model parameters to quantify uncertainty in predictions
Relevance of the problem

- Calibration of simulators has application in very many application fields, e.g.:
  - high energy physics (Higdon et al. 2005)
  - geophysics (Cui et al. 2009)
  - astrophysics (Kaufman et al. 2010)
  - industrial processes (Forrester 2010)
  - ecology (Schneider et al. 2006)
  - climatology (Guillas et al. 2004, Wilkinson 2001)
  - systems biology (Wilkinson 2010)

- quantifying uncertainty is of paramount importance for balancing risks/costs of decisions
Importance of quantifying uncertainty

- this is what we might want
  - inferring model parameters
  - obtaining predictive distributions (balance cost of decisions)
- Other desirables:
  - including prior information
  - approaching sequential estimation
  - doing model selection
Importance of quantifying uncertainty

- this is what we might want
  - inferring model parameters
  - obtaining predictive distributions (balance cost of decisions)
  - Other desirables:
    - including prior information
    - approaching sequential estimation
    - doing model selection
- Bayesian framework seems to be appropriate
Bayesian calibration of simulators

- Kennedy at al. (2001):

\[ x \xrightarrow{\text{Physical system}} z = \rho \eta(x, \theta) + \delta(x) + \varepsilon \]

\[ y \xrightarrow{\text{Simulator}} \eta(x, \theta) \]

- \( \eta(x, \theta) \) and \( \delta(x) \) independent and modeled using GPs
- \( \varepsilon \sim \mathcal{N}(0, \sigma_\varepsilon^2) \) and i.i.d.
Interpretability of calibration results

• Can we really interpret the inferred simulator parameters as the “real” ones?
• if the model differs from the physical system, then the interpretation of $\theta$ is questionable
• Model misspecification and consequences in Bayesian inference - see e.g., White (1982) and Müller (2009)
• Loeppky et al. (2006) studied the problem of model misspecification in calibration problems
Simplified calibration model - Likelihood

\[ x \rightarrow \text{Physical system} \rightarrow z = \eta(x, \theta) + \epsilon \]

\[ x \rightarrow \text{Simulator} \rightarrow y = \eta(x, \theta) \]

- we have direct access to the log-likelihood:

\[
\log[p(\text{Data}|\theta)] = \sum_i \log \left[ \mathcal{N}(z_i|\eta(x_i, \theta_i), \sigma_\epsilon^2) \right]
\]

- if we place priors \( \pi(\theta) \) we can infer \( \theta \) - simulation using Markov chain Monte Carlo (MCMC)

\[
p(\theta|\text{Data}) \propto p(\text{Data}|\theta)\pi(\theta)
\]
Given that the simulator is usually modeling a complex physical system, the likelihood is often multimodal.
Oil reservoir data

- As a working example let us consider the 2D oil reservoir model by Tavassoli et al. (2004)
- “Real” data are generated from the simulator:

\[ z_i = \eta(x_i, \tilde{\theta}) + \varepsilon_i \]

where \( \tilde{\theta} \) represents a set of “true” parameters
Inference using Metropolis-Hastings

- Poor exploration of the parameter space
- Proper exploration of the parameter space via population based Markov chain Monte Carlo (Pop-MCMC)
Inference using Pop-MCMC

• bridge from the prior to the posterior via tempering

\[
\text{tempered posterior } \propto p(\text{Data}|\theta)^t \pi(\theta)
\]

with \( t \in [0, 1] \)

• one sampler for each tempered posterior

• samplers sampling independently and exchanging samples so that invariance of \( p(\theta|\text{Data}) \) is preserved
Inference using Pop-MCMC

Metropolis–Hastings

Population MCMC

iteration

iteration

iteration

iteration

iteration

iteration

iteration

iteration

iteration
Inference using Pop-MCMC - Results

Interpretation of the multimodal posterior - throw parameter
Inference using Pop-MCMC - Results

- Graphs showing distributions of throw, khigh, and klow counts.
- Oil production rate over months with real data and mean prediction with 5th - 95th percentiles.
Inference using Pop-MCMC - Results

Oil production rate

- Real
- Mean prediction
- 5th – 95th percentiles
Inference using Pop-MCMC - Results

Oil production rate

- Real
- Mean prediction
- 5th – 95th percentiles
What if the running time of the simulator is prohibitive?

- Simulators could be so complex to require hours or even days to run
- Fully Bayesian treatment is not viable
- We aim at using the available computational resources to find parameters and an estimate of the uncertainty (not Bayesian)
Need for emulators

- Emulators as a proxy for the expensive likelihood
- Start from a set of design points (latin hypercubes)
- Emulator using Gaussian Process
Need for emulators

- Marginals of the emulator are Gaussian:
  \[ y(\theta) \sim \mathcal{N}(\mu(\theta), s^2(\theta)) \]

- Incremental design for minimization optimizing a utility (improvement) function (Jones et al. 1998)
  \[ I(\theta) = \max(f_{\text{min}} - y(\theta), 0) \]

expected value:

\[ E[I(\theta)] = (f_{\text{min}} - \mu(\theta)) \Phi \left( \frac{f_{\text{min}} - \mu(\theta)}{s(\theta)} \right) + s(\theta) \mathcal{N} \left( \frac{f_{\text{min}} - \mu(\theta)}{s(\theta)} \right) \]
Example of incremental design

![Graph showing negative log-likelihood and EI values across θ. The graph displays True, Fitted, and 5th–95th percentile lines.]
Example of incremental design

![Graph of negative log-likelihood vs. \( \theta \)]

**Graph Details:**
- **Axes:**
  - X-axis: \( \theta \)
  - Y-axis: negative log-likelihood
- **Curves:**
  - **True** (solid black line)
  - **Fitted** (dash-dot blue line)
  - **5th–95th perc** (dashed red line)

**Legend:**
- True
- Fitted
- 5th–95th perc

**Graph Elements:**
- **El:**
  - X-axis: \( \theta \)
  - Y-axis: El

**Graph Notes:**
- The graph illustrates the comparison between the true model and fitted model over the range of \( \theta \) values, showing the negative log-likelihood and the 5th–95th percentile range.
Example of incremental design
Example of incremental design
Example of incremental design

![Graph showing the relationship between negative log-likelihood and θ, with True, Fitted, and 5th-95th perc curves.]
Example of incremental design

![Graph showing negative log-likelihood and EI values over different values of θ. The graph illustrates True, Fitted, and 5th–95th percentile ranges.]
Example of incremental design

![Graph showing incremental design with negative log-likelihood](image)
Example of incremental design
Example of incremental design

[Graph showing negative log-likelihood with True, Fitted, and 5th-95th perc curves.]
Incremental design - Oil reservoir - Results

- incremental design on the oil data
- we assumed that computational resources allowed only 100 runs of the simulator
  - 50 simulations using latin hypercubes
  - 50 simulations using incremental design
Incremental design - Oil reservoir - Results

true values: 10.4, 131.6, 1.3
Incremental design - Oil reservoir - Results

true values: 10.4, 131.6, 1.3

![Graph showing the results of incremental design for an oil reservoir. The graph displays the real data points and the mean prediction along with the 5th and 95th percentiles over months. The true values for the first few months are indicated on the graph: 10.2, 123.3, and 21.9 bbl/day.](image-url)
Incremental design - Oil reservoir - Results

true values: 10.4, 131.6, 1.3

![Graph showing bbl/day vs months with real data, mean prediction, and 5th-95th percentiles. The graph includes a tick mark at 0, 20, 40, 60, 80, 100, 120 months on the x-axis and bbl/day on the y-axis. The true values are indicated as 46.76 (37.47), 122.07 (3.37), 19.85 (8.65).]
Conclusions and ongoing work

• This work is part of the ongoing research program of the Computational Statistics group at UCL on inference in complex systems
• Calibration of simulators is an important and promising research area
• It is a challenging problem even with simplifying assumptions:
  • inference over parameters of complex simulators
  • expensive to evaluate the likelihood
Conclusions and ongoing work

Ongoing research:

• Composite likelihoods
• Emulators for moderate/large sized data sets
• Consistency of estimators in incremental experiment design?
• Hybrid/Manifold Monte Carlo with emulator as potential field
• Design of covariance functions for emulators of differential equations based simulators
• Model selection
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